Advances in the MaryLie/IMPACT (ML/I) beam dynamics code

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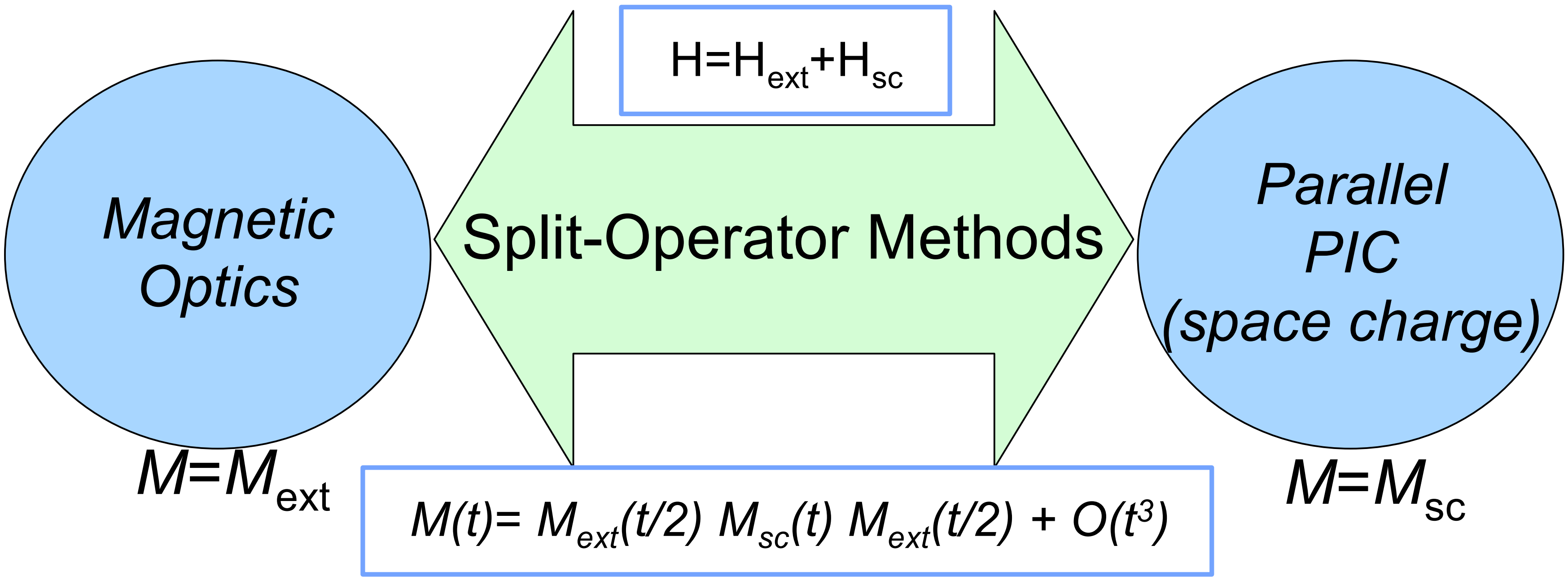
ComPASS project meeting
Dec 2, 2008

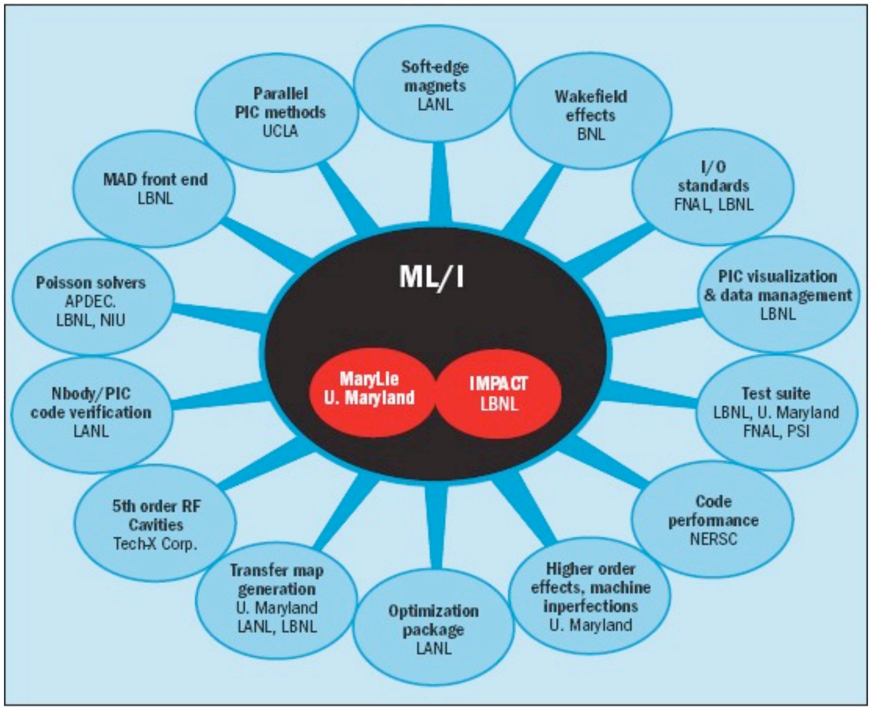
MaryLie/IMPACT uses a split-operator approach to combine high-order optics with parallel PIC



- **Note that the rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields**
- **Leads to extremely efficient particle advance:**
  - **Do not take tiny steps to push ~100M particles**
  - **Do take tiny steps to compute maps; then push particles w/ maps**

MaryLie/IMPACT (ML/I)

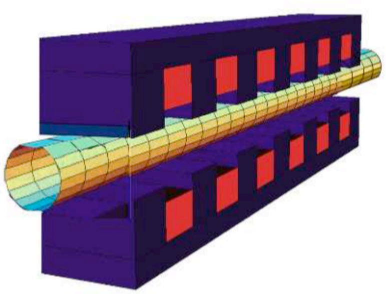
- Combines capabilities of MaryLie code (from U. Md.) with IMPACT code (from LBNL) + new features
- Multiple capabilities in a single unified environment:
  - Map generation
  - Map analysis
  - Particle tracking w/ 3D space charge
  - Envelope tracking
  - Fitting and optimization

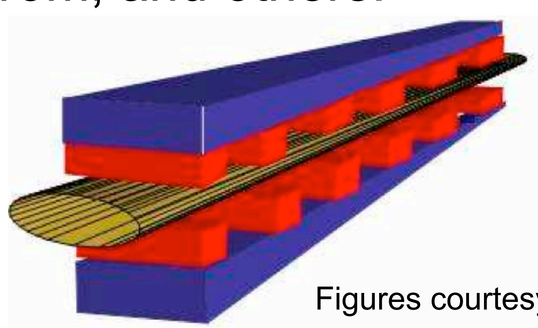


- Parallel
- 5th order optics
- 3D space charge
- 5th order rf cavity model
- 3D integrated Green function
- Photoinjector modeling
- Soft-edged magnets
- Coil stacks
- MAD-style input compatibility
- “Automatic” commands
- Test suite

5th order RF cavity model

- **Numerical generation of xfer maps for rf cavities described in 1995**
  - R. Ryne, “The linear map for an RF gap including acceleration, LANL Technical Note (1995)
  - R. Ryne, “Finding matched rms envelopes in rf linacs: A Hamiltonian approach,” acc-phys/9502001 (1995).
  - J. van Zeijts, “Arbitrary order transfer maps for RF cavities,” PAC 1995
- **Linear version implemented in IMPACT in 1995 (R. Ryne)**
- **5th order version implemented in MaryLie/IMPACT in 2006 (D. Abell)**
  - D. Abell, Numerical computation of high-order transfer maps for rf cavities, PRST-AB 9, 052001 (2006).
- **Abell paper includes methodology for generation of high order rf cavity generalized gradients from field data**
  - Extends approach previously developed for magnetostatic elements by Dragt, Venturini, Walstrom, and others.





Figures courtesy Alex Dragt, U. Md.

Integrated Green Function

- Addresses the issue that certain convolution-based Poisson solvers have very poor accuracy when the grid aspect ratio is large
- 2D version w/ linear basis functions described at 2003 ICFA workshop on space-charge simulation, implemented in ML/I
- Independently developed by Ryne (2003), Ohmi (2000), and Ivanov (1989)

Observations

- The Green function, G, and source density, ρ, may change over vastly different scales
- G is known apriori; ρ is not

> We should use all the information available regarding G so that the numerical solution is <u>only limited by our approximate knowledge of ρ</u>

- Example: 2D Poisson equation in free space

$$\phi(x,y) = \int G(x-x',y-y')\rho(x',y')dx'dy'$$

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Standard Approach (Hockney and Eastwood)

$$\phi_{i,j} = \sum G_{i-i',j-j'}\rho_{i',j'}$$

- This approach is equivalent to using the trapezoidal rule (modulo treatment of boundary terms) to approximate the convolution integral
- This approach makes use of only partial knowledge of G
- The error depends on how rapidly the integrand, ρG, varies over an elemental volume
  - If ρ changes slowly we might try to use a large grid spacing; but this can introduce huge errors due to the change in G over a grid length

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Integrated Green Function, cont.

- Assume the charge density, ρ, varies in a prescribed way in each cell
- Use the analytic form of the Green function to perform the convolution integral <u>exactly</u> in each cell, then sum over cells
- Example: linear basis functions to approximate ρ in a cell:

$$\phi(x_i,y_j)=\sum_{i',j'}\rho_{i,j}\int_0^{h_x}dx'\int_0^{h_x}dy'(h_x-x')(h_y-y')G(x_i-x_{i'}-x',y_j-y_{j'}-y')+$$

$$\sum_{i',j'}\rho_{i+1,j}\int_0^{h_x}dx'\int_0^{h_x}dy'x'(h_y-y')G(x_i-x_{i'}-x',y_j-y_{j'}-y')+$$

$$\sum_{i',j'}\rho_{i,j+1}\int_0^{h_x}dx'\int_0^{h_x}dy'(h_x-x')y'G(x_i-x_{i'}-x',y_j-y_{j'}-y')+$$

$$\sum_{i',j'}\rho_{i+1,j+1}\int_0^{h_x}dx'\int_0^{h_x}dy'x'y'G(x_i-x_{i'}-x',y_j-y_{j'}-y')$$

- Shifting the indices results in a single convolution involving an integrated effective Green function: $\phi_{i,j}=\sum G^{eff}_{i-i',j-j'}\rho_{i',j'}$

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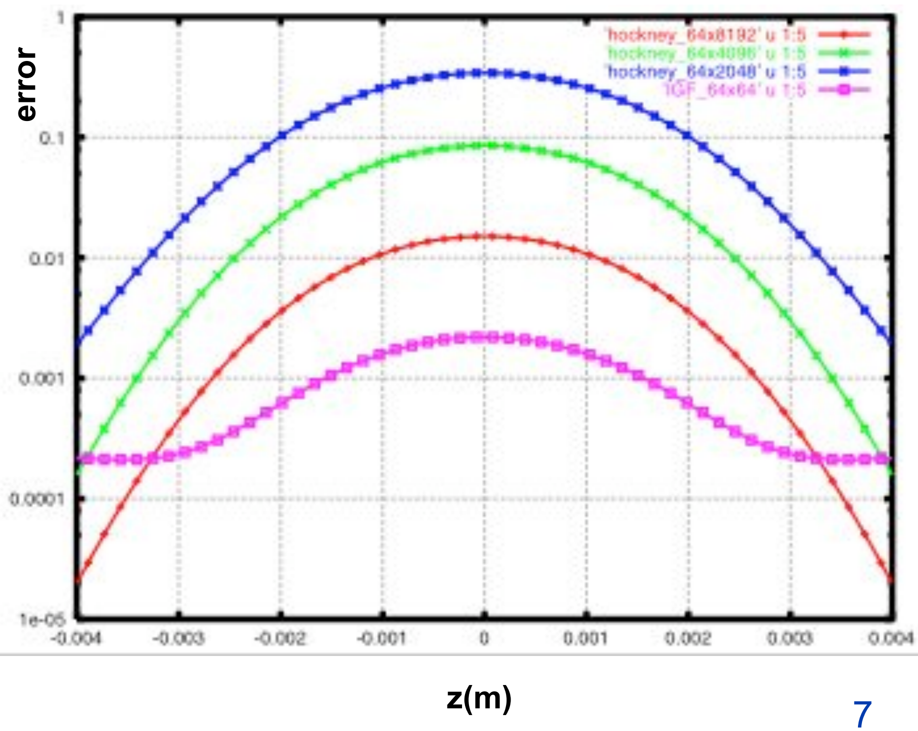
Integrated Green Function: Status in the ComPASS project

- 3D Version w/ linear basis functions implemented in ML/I (D. Abell)
  - Quad precision version now running on Franklin via D. Bailey's DDFUN package
- 3D Version w/ constant basis functions implemented in IMPACT (J. Qiang)
- 2D Version w/ constant basis functions implemented in BeamBeam3D (J. Qiang)
- Qiang has also invented a shifted IGF for use in computing beam-beam interactions

Example: Error in electric field computed using different algorithms applied to a 2D Gaussian elliptical density distribution w/ 500:1 aspect ratio

Hockney: 64x2048, 64x4096, 64x8192
IGF: 64x64



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- J. Qiang, S. Lidia, R. Ryne, C. Limborg-Deprey, "3D quasistatic model for high brightness beam dynamics simulation," Phys. Rev. ST Accel. Beams 9, 044204 (2006). See also Erratum, Phys. Rev. ST Accel. Beams 10, 129901 (2007).
- J. Qiang, M. Furman, R. Ryne, "A parallel particle-in-cell model for beam-beam interation in high energy ring colliders," J. Comp. Phys. 198, 1, pp. 278-294 (July 2004)
- K. Ohmi,"Simulation of beam-beam effects in a circular e^+e^- collider," Phys. Rev. E 62, 2000, pp. 7287-7294.
- V. Ivanov, "Numerical methods for analysis of 3D non stationary flows of charged particles," 15 Trudy Instituta Matematiki, Izd-vo "Nauka," Sibirskoe Otdelenie, pp. 172-187 (1989).

ML/I photoinjector capability: Issues

- Z-code or T-code?
  - Z-codes need to convert from "coordinates at fixed z" to "coordinates at fixed t" for each space-charge calc since Poisson is solved at fixed t
  - Z-codes have difficulty w/ space charge unless trajectories are approx linear over a distance equal to the bunch length
    - Could probably use a z-code for a photoinjector, but no one would believe the result unless checked against a t-code. So we've implemented a t-code
- Symplectic or Non-symplectic?
  - Symplectic methods essential for studying long-term behavior in circular accelerators. But photoinjector does not involve long-term simulation
    - I don't expect symplecticity to be essential for photoinjector modeling
    - Other factors might be more important, e.g. adjustable step size for high accuracy near the cathode. So we've implemented non-symplectic approach
- Conclusion: use time-based, non-symplectic approach:
  - Numerical simulation of the Lorentz force equations for $\zeta(t)$ where $\zeta = (x, \gamma\beta_x, y, \gamma\beta_y, z, \gamma\beta_z)$

Numerical Integration Algorithm

- Integrate particle trajectories using adjustable step Runge-Kutta
  - Pros: easy to implement
  - Cons:
    - uses a lot of memory for temporary vectors (but low storage RK4 might help)
    - Extra space-charge calculations
- Current implementation uses 4th order or 8th order
  - First integrate w/ time step h; then integrate w/ two steps of size h/2
    - The difference can be used for error control:
      - If difference exceeds ε_1, cut step size in half and repeat
      - If difference is below ε_2,
        - » time step is a success
        - » double step size for next step

RK Error Control

- Straightforward when space charge is absent
  - —Base on a single (representative) particle; or maximum over all particles; or average over particles; other choices…
- More complicated when space charge is present
  - Numerical noise in particle-based Poisson solver is problematic
- Current implementation takes a pragmatic approach:
  - —Choose a method for error control when space charge is absent
  - —Adapt to include space charge; should approach zero-current method as space charge tends to zero
  - —When space charge is present, will need to repeat runs with reduced error threshold to verify convergence

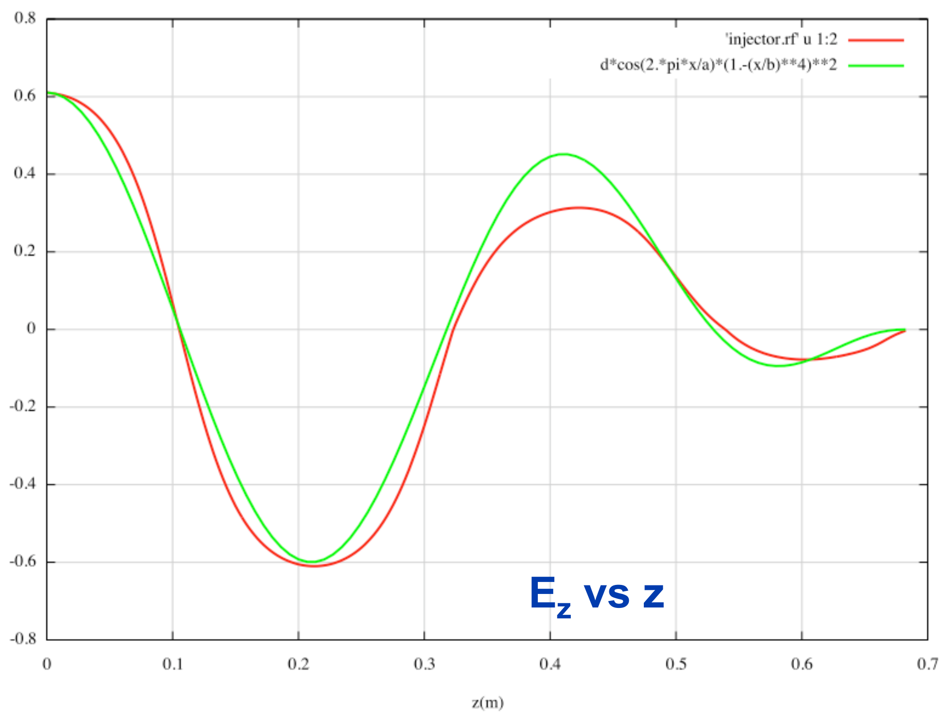
Presently, we use the energy gain of a single particle to determine error associated with a step. We save the space-charge force on this particle at the start of the step and assume it is constant throughout the step. As a result, intra-step space-charge noise is not an issue.

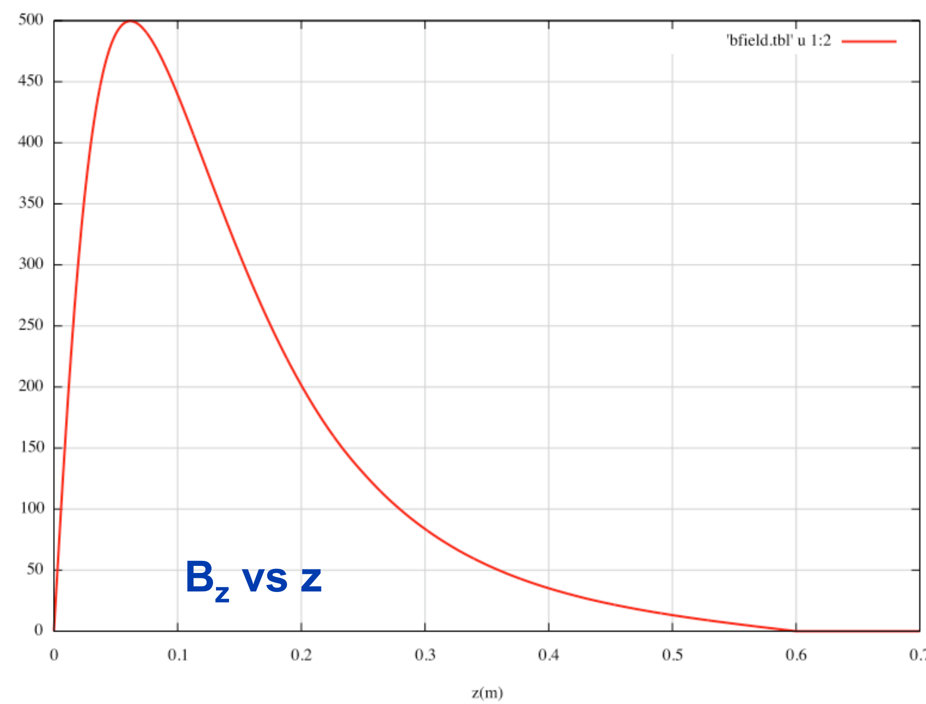
Poisson Solver

- Use doubled grid convolution (“Hockney algorithm”) to compute space charge subject to open boundary conditions
  - —Standard algorithm fails badly due to extreme aspect ratio of the bunch near the cathode
    - Grid cell length ~100x smaller than transverse cell size
- Use Integrated Green function technique to solve the aspect ratio problem
  - —Likely need quad precision if grid aspect ratio > 100
- Image charges of infinite plane cathode included via equal and opposite image charges behind the cathode

Application

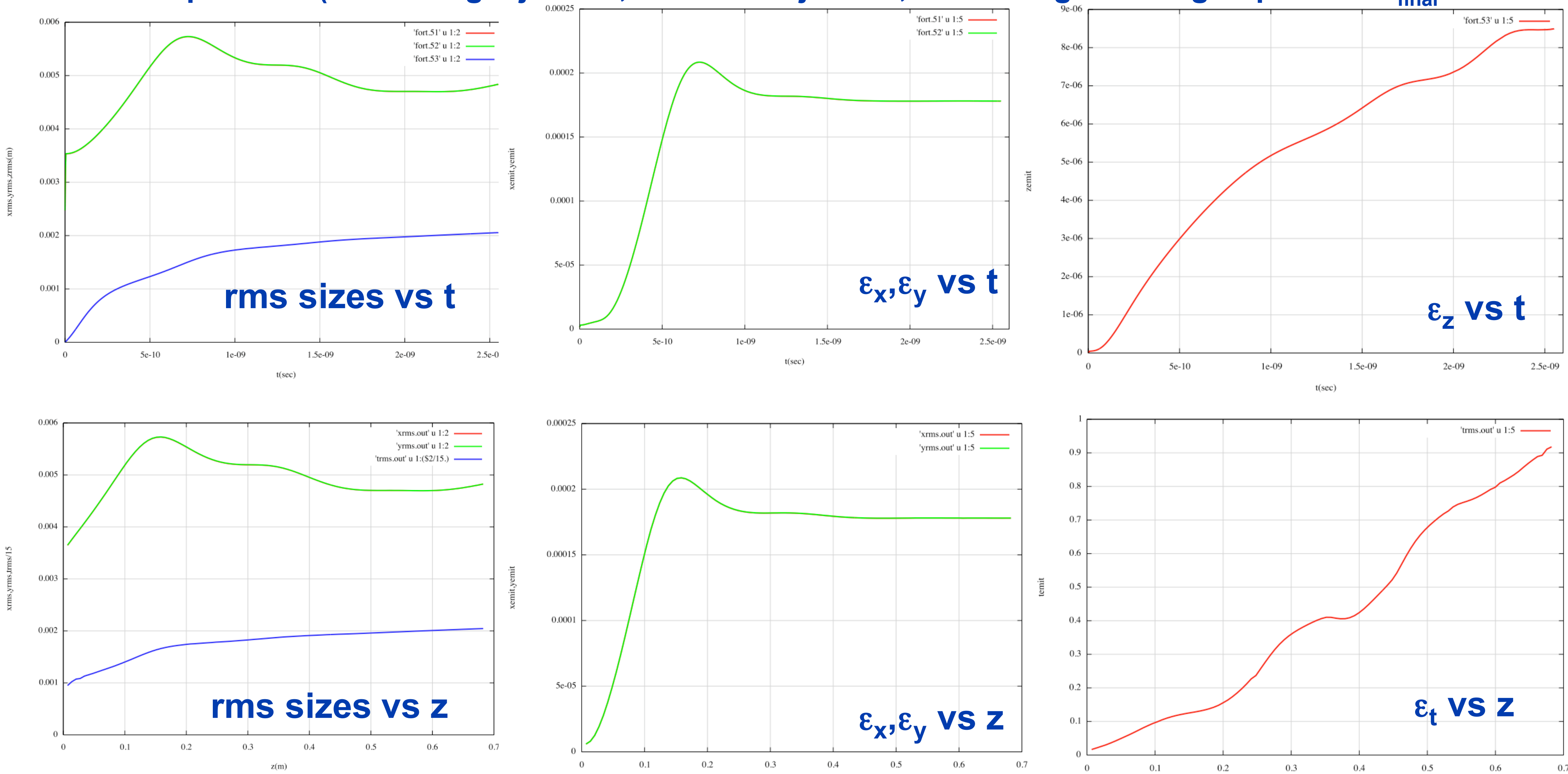
- Test Example:
  - — 1 nC, 700 MHz, E_{final}=2.7 MeV
  - — Cathode radius=7 mm, $E_{emission}$= 0-1 eV, $\Delta\phi$=2.5 deg
- Simulation parameters: 8M particles, 32x32x512 grid. Error control:
  - — if error >10^{-10}, cut time step (Δt) in half and repeat step
  - — if 10^{-10} < error < 10^{-11}, step was successful; leave Δt unchanged
  - — if error < 10^{-11}, step was successful; double Δt for next step





RMS quantities vs t; RMS quantities vs z

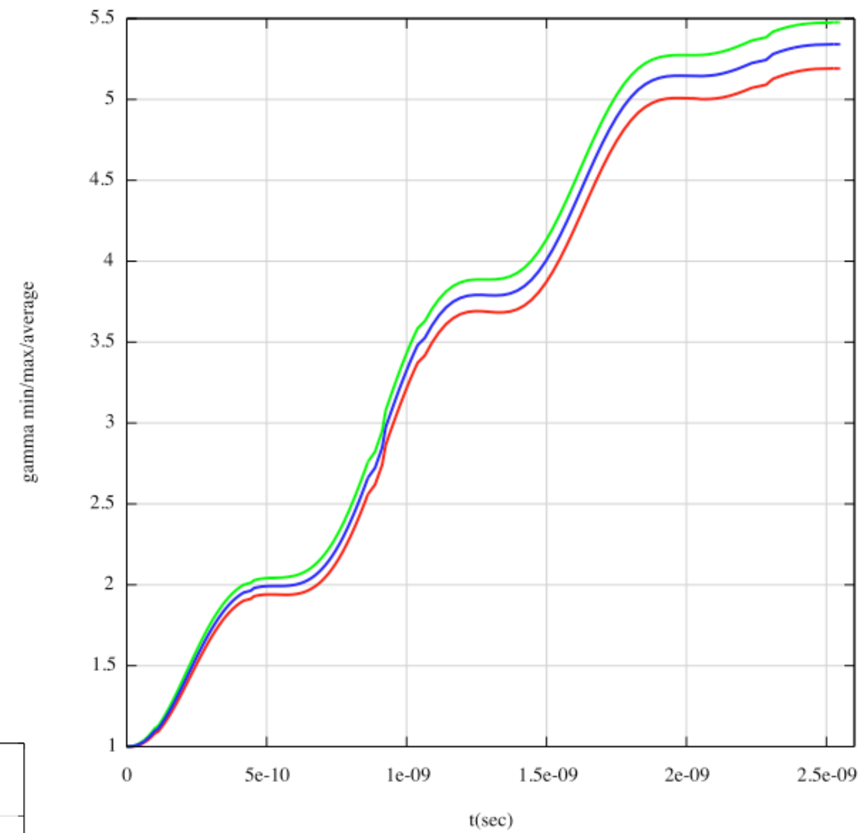
Diagnostics vs t produced at each time step of the RK integrator (no extrapolation required). Total # of steps = 533 (100 during injection, 333 after injection, 100 during crossing of plane at z_{final}



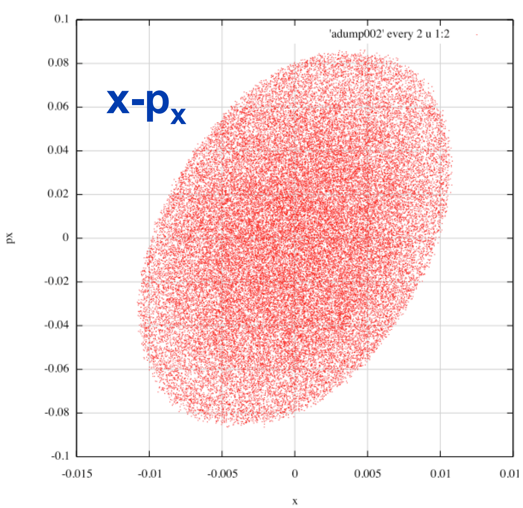
Diagnostics produced by first constructing a longitudinal (z) grid, accumulating particles as they advance in time when they cross z-grid points, using 1-step Euler over a fraction of a time step to estimate coordinates at z-crossing point.

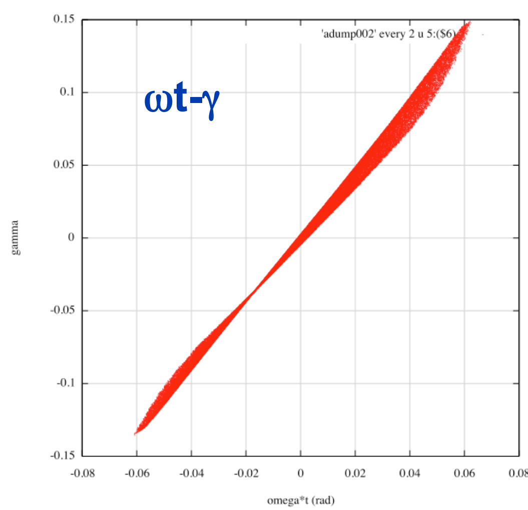
Evolution of energy spread; final phase space

- Gamma values at end of injector:
  - γ_{min}=5.190574164
  - γ_{max}=5.476896407
  - $<\gamma>$=5.340775754
  - $<E_{kin}>$=2.218107 MeV
  - $<E_{tot}>$=2.729107 MeV



Final phase space





Future Plans

- Strengthen capability for modeling space-charge in rings
- Strengthen capability for modeling ultra-low losses
- Complete domain decomposition version of ML/I
- Complete development of photoinjector module and distribute to other ComPASS members
- Implement new capabilities, as needed, for HEP and NP priorities